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4. TITLE AND SUBTITLE Computational and Theoretical Investigations of Strongly Correlated Fermions in Optical Lattices				5a. CONTRACT NUMBER W911NF-08-1-0338	
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6. AUTHORS Mohit Randeria, Nandini Trivedi				5d. PROJECT NUMBER	
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14. ABSTRACT This proposal brings together unique expertise in Quantum Monte Carlo and analytical techniques to address problems that are at the cutting edge of research in strongly correlated atomic fermions in optical lattices. (1) For fermions with attractive interactions, the possibility of a pseudogap phase, that shows signatures of pairing but no long range phase coherence, in an unequal population of "up" and "down" fermions is investigated. (2) For					
15. SUBJECT TERMS fermions, optical lattices, strong correlations, quantum Monte Carlo, pseudogap phase, d-wave superfluids, antiferromagnets, Hubbard models, quantum phase transitions					
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Report Title

Computational and Theoretical Investigations of Strongly Correlated Fermions in Optical Lattices

ABSTRACT

This proposal brings together unique expertise in Quantum Monte Carlo and analytical techniques to address problems that are at the cutting edge of research in strongly correlated atomic fermions in optical lattices. (1) For fermions with attractive interactions, the possibility of a pseudogap phase, that shows signatures of pairing but no long range phase coherence, in an unequal population of “up” and “down” fermions is investigated. (2) For fermions with repulsive interactions, the evidence for a d-wave superfluid ground state is analysed, especially its competition with spin liquid and antiferromagnetic phases. Progress on both of these questions will impact not only the fields of cold atoms and condensed matter of strongly correlated systems, but also complex transition metal oxides. Issues related to thermometry, inhomogeneous trap potentials and effects of thermal and quantum phase fluctuations, that are central for an accurate interpretation of experiments, are investigated. A combination of variational, Green function and determinantal quantum Monte Carlo simulations, Bogoliubov deGennes theory, and functional integral methods will be implemented to address the variety of issues highlighted above. The detailed comparisons between simulations, theory and experiments is crucial for validation of the results. These methods are essential to calculate properties in regimes where standard paradigms break down and the phenomena are non-perturbative. The proposed research program is strongly motivated by current experiments and has the potential to guide future ones. Ultimately, the goal is to establish new paradigms for strongly correlated fermion systems.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

<u>Received</u>	<u>Paper</u>
03/04/2013	3.00 Nandini Trivedi, Yen Lee Loh. Detecting the Elusive Larkin-Ovchinnikov Modulated Superfluid Phases for Imbalanced Fermi Gases in Optical Lattices, Physical Review Letters, (04 2010): 0. doi: 10.1103/PhysRevLett.104.165302
03/04/2013	2.00 H. Krishnamurthy, Yasuyuki Kato, Naoki Kawashima, Nandini Trivedi, J. Freericks. Strong-coupling expansion for the momentum distribution of the Bose-Hubbard model with benchmarking against exact numerical results, Physical Review A, (05 2009): 0. doi: 10.1103/PhysRevA.79.053631
03/04/2013	4.00 Mohit Randeria, William Schneider. Universal short-distance structure of the single-particle spectral function of dilute Fermi gases, Physical Review A, (02 2010): 0. doi: 10.1103/PhysRevA.81.021601
03/04/2013	5.00 Thereza Paiva, Richard Scalettar, Mohit Randeria, Nandini Trivedi. Fermions in 2D Optical Lattices: Temperature and Entropy Scales for Observing Antiferromagnetism and Superfluidity, Physical Review Letters, (02 2010): 0. doi: 10.1103/PhysRevLett.104.066406
03/04/2013	6.00 Roberto B. Diener, Mohit Randeria. BCS-BEC crossover with unequal-mass fermions, Physical Review A, (03 2010): 0. doi: 10.1103/PhysRevA.81.033608
03/04/2013	7.00 Mohit Randeria, Edward Taylor. Viscosity of strongly interacting quantum fluids: Spectral functions and sum rules, Physical Review A, (05 2010): 0. doi: 10.1103/PhysRevA.81.053610
03/04/2013	8.00 Mohit Randeria. Ultracold Fermi gases: Pre-pairing for condensation, Nature Physics, (08 2010): 0. doi: 10.1038/nphys1748
03/04/2013	9.00 S.-Y. Chang, M. Randeria, N. Trivedi. Ferromagnetism in the upper branch of the Feshbach resonance and the hard-sphere Fermi gas, Proceedings of the National Academy of Sciences, (12 2010): 0. doi: 10.1073/pnas.1011990108
03/04/2013	10.00 Thereza Paiva, Yen Lee Loh, Mohit Randeria, Richard T. Scalettar, Nandini Trivedi. Fermions in 3D Optical Lattices: Cooling Protocol to Obtain Antiferromagnetism, Physical Review Letters, (08 2011): 0. doi: 10.1103/PhysRevLett.107.086401
03/04/2013	11.00 Edward Taylor, Shizhong Zhang, William Schneider, Mohit Randeria. Colliding clouds of strongly interacting spin-polarized fermions, Physical Review A, (12 2011): 0. doi: 10.1103/PhysRevA.84.063622
03/04/2013	12.00 Mason Swanson, Yen Lee Loh, Nandini Trivedi. Proposal for interferometric detection of the topological character of modulated superfluidity in ultracold Fermi gases, New Journal of Physics, (03 2012): 0. doi: 10.1088/1367-2630/14/3/033036
03/04/2013	13.00 Roberto Diener, Rajdeep Sensarma, Mohit Randeria. Quantum fluctuations in the superfluid state of the BCS-BEC crossover, Physical Review A, (02 2008): 0. doi: 10.1103/PhysRevA.77.023626
03/04/2013	14.00 Qi Zhou, Yasuyuki Kato, Naoki Kawashima, Nandini Trivedi. Direct Mapping of the Finite Temperature Phase Diagram of Strongly Correlated Quantum Models, Physical Review Letters, (08 2009): 0. doi: 10.1103/PhysRevLett.103.085701
08/27/2013	15.00 E. Duchon, Y. Kato, N. Trivedi. Diagnostic for phases and quantum critical regions using deviations from the local fluctuation-dissipation theorem, Physical Review A, (12 2012): 0. doi: 10.1103/PhysRevA.86.063608

TOTAL: 14

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

<u>Received</u>	<u>Paper</u>
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TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

1. Invited talk on Bosons in optical lattices: Mapping the phase diagram of the Finite Temperature Bose Hubbard Model at the International Conference on "Frontiers of Degenerate Quantum Gases", Center of Advanced Study of Tsinghua University (CASTU), Beijing, October 20-24, 2008.
2. Invited talks at "School on Correlated Systems", organized by the Tata Institute of Fundamental Research at Mahabaleshwar, India, December 2008.
3. Invited talk on Bose and Fermi Hubbard Models: Achievements and Challenges at the Optical Lattice Emulator meeting, Las Vegas, Dec 15-18, 2008.
4. Seminar on Bosons in optical lattices: Mapping the phase diagram of the Bose Hubbard Model, Purdue University, September 5, 2008
5. Invited speaker at conference Superconductivity: from collective modes to quantum phase transitions, "Supergold" conference celebrating Allen Goldmans career, Minneapolis, May 1-3, 2009. Talk title: Cold Atoms Meets Condensed Matter Physics
6. Speaker at "SummerWorkshop on Quantum Vortices and Fluctuations in Superconductors and Superfluids", July 6-24, 2009.
7. Discussion leader at "Recent progress in many body theories 15", The Ohio State University, Columbus, OH, July 27-31, 2009.
8. Invited speaker at the "International Symposium on Quantum Fluids and Solids - QFS2009, Northwestern University, August 5-12, 2009. Talk title: The not so elusive Larkin-Ovchinnikov phase for Imbalanced Fermi Gases in Optical Lattices
9. Invited speaker at Condensed Matter Physics of Cold Atoms Program at KITPC/ITP-CAS, Beijing, October 12-19, 2009. Talk title: Strong Correlation Effects in the Normal State of Bose and Fermi Gases in Optical Lattices from unbiased Quantum Monte Carlo Simulations
10. Invited speaker at workshop on "ab-initio modeling of cold gases", CTS/Cecam/QSIT, Nov 11-13, Zurich. Talk title: Single atom addressability and mapping the finite temperature phase diagram of the Bose Hubbard Model from unbiased Quantum Monte Carlo Simulations
11. Invited talk on "Detection of modulated superfluid phases", at Optical Lattice Emulator/DARPA meeting, December 2-3, Miami, 2009.
12. Colloquium on Cold Atoms Meets Condensed Matter Physics, University of Illinois, Chicago, April 15, 2010
13. Colloquium on Cold Atoms in Optical Lattices: Challenges to mapping out quantum phase transitions, Texas A&M, March 4, 2010
14. Seminar on "Hubbard type models and Cold Atoms in optical lattices", Tata Institute of Fundamental Research, Mumbai, December 8, 2010

15. Seminar on "The not so elusive Larkin-Ovchinnikov phase for Imbalanced Fermi Gases in Optical Lattices", Rice University, March 3, 2010
16. Invited speaker, workshop on "Exotic Insulating Phases of Quantum Matter", The Johns Hopkins University, January 14-16, 2010.
17. Discussion Leader, Gordon Research Conference on "Correlated Electron Systems", June 13-17, 2010, Mount Holyoke College, South Hadley, MA.
18. Invited Lecturer, Boulder Summer School, "Computational and conceptual approaches to quantum many-body systems" in July 5-30, 2010, University of Colorado, Boulder.
19. Invited speaker, "Frontiers of Ultracold Atoms and Molecules", Oct 11-15, 2010, Kavli Institute of Theoretical Physics, Santa Barbara, CA, talk titled "Simulations and Emulations of Fermions in Optical Lattices".
20. Invited speaker, "Disentangling Quantum Many-body Systems: Computational and Conceptual Approaches", Kavli Institute of Theoretical Physics, Santa Barbara, CA, October 31 November 12, 2010.
21. Invited speaker, "Physics of Superconductor-Insulator Transition and related topics", Argonne National Laboratory, November 16-19, 2010; talk titled "Single and two-particle spectral functions across the disorder-driven superconductor- insulator transition".
22. Invited speaker, "Fermions in Optical Lattices: Cooling Protocol to Observe Antiferromagnetism", APS March Meeting, March 21-25, 2011, Dallas, TX.
23. Colloquium on Cold Atoms in Optical Lattices: Challenges to mapping out quantum phase transitions, University of Kentucky, February 4, 2011.
24. Seminar on "Strongly Interacting Fermions and Bosons: Quantum Monte Carlo (QMC) simulations", Optical Lattice Emulator, DARPA Meeting, Houston TX, May 24, 2010.
25. Seminar on "Detection of novel (and not so novel) phases in optical lattices", MIT-Harvard Center of Ultracold Atoms, October 5, 2010, MIT.
26. Seminar on "Single and two-particle energy gaps across the disorder-driven superconductor- insulator transition", October 7, 2010, Harvard.
27. Seminar on "Probing Quantum Phases of Matter in Optical Lattices", State University of New York, Stony Brook, NY, February 25, 2011.
28. Seminar on "Mapping the finite temperature phase diagram of the Bose Hubbard Model from unbiased Quantum Monte Carlo Simulations", NIST, April 16, 2010, Maryland.
29. Invited speaker, Workshop on "Superconductivity:100 years young",

Natal, Brasil, May 16-27 (2011).

30. Invited speaker, "Workshop on Frontiers in Ultracold Fermi Gases", ICTP, Trieste, Italy, June 6 -10 (2011).

31. Speaker at "Optical Lattice Emulator" DARPA Program", on "Quantum Monte Carlo (QMC) simulations of Strongly Interacting Fermions and Bosons", Vail, CO, June 20-23, 2011.

32. Invited talk "Ferromagnetism" at the "Winter school and workshop on spin physics and topological effects in cold atoms, condensed matter, and beyond", College Station, TX, December 12-17, 2011.

33. Colloquium on Cold Atoms meets Condensed Matter Physics, Northwestern University, April 22, 2011.

34. Colloquium on Cold Atoms in Optical Lattices: Challenges to emulating real materials, Tata Institute of Fundamental Research, Mumbai, India, July 10, 2011.

35. Colloquium on Cold Atoms in Optical Lattices: Challenges to mapping out quantum phase transitions, McGill University, October 7, 2011.

36. Colloquium on High Temperature Superconductivity and the Optical Lattice Emulator, Perimeter Institute, November 14, 2011.

37. Seminar on "Single and two-particle energy gaps across the disorder-driven superconductor- insulator transition, Northwestern University, April 21, 2011.

38. Seminar on "Unusual Modulated Superfluid states in unbalanced atomic gases", Tata Institute of Fundamental Research, July, 2011.

39. Invited speaker, "Fermions in Optical Lattices: Status of the Optical Lattice Emulator Program", DARPA OLE Meeting, May 31, 2012.

40. 15 lectures at Perimeter Scholars International, Perimeter Institute, Waterloo, November 2011.

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MOHIT RANDERIA

Three Lectures on "Cold Atoms and Strongly Correlated Superconductors" at the "School on Correlated Systems", organized by the Tata Institute of Fundamental Research at Mahabaleshwar, India, December 2008.

"BCS-BEC crossover and the unitary Fermi gas", Invited Lecture at the International Conference in Recent Progress in Many Body Theories, Columbus, Ohio, July 2009.

Colloquium on "Ultracold Atomic Gases" at Kenyon College, Ohio, April 2010.

Invited Talks on (i) "Viscosity of strongly interacting quantum Fluids" and (ii) "Ferromagnetism in dilute Fermi gases" at Canadian Institute for Advanced Scientific Research (CIFAR) Conference, Montreal, May 2010.

Invited Lecture on "BCS-BEC crossover and the Unitary Fermi Gas" at the Canadian Institute for Advanced Scientific Research (CIFAR) Summer School, Montreal, May 2010.

Invited Lecture on “Viscosity of strongly interacting quantum fluids” at the Condensed Matter Interaction Meeting, University of Cincinnati, May 2010.

(i) Five Lectures [jointly with T. Senthil (MIT)] on “Doped Mott Insulators and High Tc Superconductivity” and (ii) Lecture on “Viscosity of strongly interacting quantum gases” at the International Center of Theoretical Sciences Winter School and Conference, Mysore, India, December 2010.

“Pseudogap and RF spectroscopy in strongly interacting Fermi gases”, Invited Talk at “Fermions from Cold Atoms to Neutron Stars: Benchmarking the Many-Body Problem”, Conference at the Institute for Nuclear Theory (INT), Washington, Seattle, May 2011.

“Viscosity of strongly interacting Fermi gases”, JILA Colloquium, JILA, University of Colorado, November 2011.

“Viscosity of strongly interacting Fermi gases”, Physics Colloquium, Harvard University, November 2011.

Lecture Course of 8 lectures on Superconductivity, Superfluidity, and Strong Correlations at the International Center of Theoretical Sciences (ICTS) Winter School on Strongly Correlated Systems at the Indian Institute of Science, Bangalore, December 2011.

“Viscosity of strongly interacting Fermi gases”, Invited talk at the International Center of Theoretical Sciences (ICTS) Conference on Strongly Correlated and Disordered Systems, IISc., Bangalore, December 2011.

“Viscosity of strongly interacting Fermi gases”, Invited Talk at the International Conference on Cold Atoms, Hong Kong, May 2012.

“Viscosity of strongly interacting Fermi gases” Physics Colloquium, Boston College, April 2012.

“BCS-BEC Crossover and the Unitary Fermi Gas”, Physics and Astronomy Colloquium, Case Western Reserve University, February 2012.

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

<u>Received</u>	<u>Paper</u>
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TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

<u>Received</u>	<u>Paper</u>
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TOTAL:

(d) Manuscripts

<u>Received</u>	<u>Paper</u>
08/27/2013	18.00 Thereza Paiva, Richard Scalettar, Mohit Randeria, Nandini Trivedi. Fermions in 2D Optical Lattices: Temperature and Entropy Scales for Observing Antiferromagnetism and Superfluidity, PHYSICAL REVIEW LETTERS (06 2009)
08/27/2013	19.00 Thereza Paiva, Yen Lee Loh, Mohit Randeria, Richard T. Scalettar, Nandini Trivedi. Fermions in 3D Optical Lattices: Cooling Protocol to Obtain Antiferromagnetism, Physical Review Letters (05 2011)
08/27/2013	16.00 K. W. Mahmud, E. N. Duchon, Y. Kato, N. Kawashima, R. T. Scalettar, N. Trivedi. Finite-temperature study of bosons in a two-dimensional optical lattice, Physical Review B (08 2011)
08/27/2013	17.00 . Direct Mapping of the Finite Temperature Phase Diagram of Strongly Correlated Quantum Models, Physical Review Letters (accepted) (03 2009)
08/27/2013	20.00 Yen Lee Loh, Nandini Trivedi, Mason Swanson. Proposal for interferometric detection of the topological character of modulated superfluidity, interference, ultracold Fermi gases, New Journal of Physics (09 2011)
08/27/2013	21.00 Yen Lee Loh, Nandini Trivedi. Detecting the Elusive Larkin-Ovchinnikov Modulated Superfluid Phases for Imbalanced Fermi Gases in Optical Lattices, Physical Review Letters (09 2009)
08/27/2013	22.00 M Jiang, R Nanguneri, N Trivedi, G G Batrouni, R T Scalettar. Gapless inhomogeneous superfluid phase with spin-dependent disorder, New Journal of Physics (10 2012)
08/27/2013	23.00 William S. Cole, Shizhong Zhang, Arun Paramekanti, Nandini Trivedi. Bose-Hubbard Models with Synthetic Spin-Orbit Coupling: Mott Insulators, Spin Textures, and Superfluidity, Physical Review Letters (05 2012)
08/27/2013	24.00 Sandeep Pathak, Nandini Trivedi, Soon Yong Chang. Repulsive fermions in optical lattices: Phase separation versus coexistence of antiferromagnetism and d-wave superfluidity, Physical Review A (12 2011)
08/27/2013	25.00 Soon Yong Chang, Mohit Randeria, Nandini Trivedi. Ferromagnetism in the upper branch of the Feshbach resonance and the hard-sphere Fermi gas, Proceedings National Academy of Sciences (08 2010)
08/27/2013	26.00 William Schneider, Mohit Randeria. Universal short-distance structure of the single-particle spectral function of dilute Fermi gases, Physical Review A (03 2010)
08/27/2013	27.00 Vijay B. Shenoy, Mohit Randeria, William Schneider. Theory of Radio Frequency Spectroscopy of Polarized Fermi Gases, ArXiv: 0903.3006 (03 2009)
08/27/2013	28.00 Roberto B. Diener, Mohit Randeria. BCS-BEC crossover with unequal-mass fermions, Physical Review A (03 2010)

08/27/2013 29.00 Edward Taylor, Mohit Randeria. Viscosity of strongly interacting quantum fluids: Spectral functions and sum rules,
PHYSICAL REVIEW A 81, 053610 (2010) (02 2010)

08/27/2013 30.00 Mohit Randeria. Ultracold Fermi gases: Pre-pairing for condensation,
Nature Phys. 6, 561 (2010) (08 2010)

08/27/2013 31.00 Edward Taylor, Shizhong Zhang , William Schneider, Mohit Randeria. Colliding clouds of strongly interacting spin-polarized fermions,
PHYSICAL REVIEW A 84, 063622 (2011) (07 2011)

TOTAL: 16

Number of Manuscripts:

Books

Received Paper

TOTAL:

Patents Submitted

Patents Awarded

Awards

Nandini Trivedi, Fellow of the American Physical Society

Graduate Students

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	Discipline
Eric Duchon	0.13	
Matthew Timothy Warren	0.08	
FTE Equivalent:	0.21	
Total Number:	2	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
Roberto Diener	0.10
Karim Bouadim	0.50
Edward Taylor	0.21
Shizhong Zhang	0.19
FTE Equivalent:	1.00
Total Number:	4

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	National Academy Member
Mohit Randeria	0.12	
Nandini Trivedi	0.09	
FTE Equivalent:	0.21	
Total Number:	2	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	Discipline
Joseph Landon Garrett	0.07	Physics
Thomas Preston Hinkle	0.04	Physics
FTE Equivalent:	0.11	
Total Number:	2	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 1.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 1.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 1.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 1.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: 1.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME

PERCENT SUPPORTED

FTE Equivalent:

Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

1 Introduction

Ultracold atomic gases have emerged as excellent laboratories for gaining insights into strongly interacting quantum fluids and correlated quantum materials. During the period funded by ARO, the PI's have made several important and significant theoretical contributions (evidenced by the high profile contributions in PNAS and Physical Review Letters) and elucidated the physics of strongly interacting Bose and Fermi gases, as well as problems at the interface of quantum gases and condensed matter physics, motivated by exciting new experiment developments.

The research has built on our complementary strengths of the PIs combining both quantum Monte Carlo (QMC) simulations and analytical approaches and this has greatly enhanced insights gained from the investigations and the value of the publications. Their flexibility and broad range of approaches have allowed the PIs to attack the most challenging problems raised by new experiments.

Technology Transfer

Computational and Theoretical Investigations of Strongly Correlated Fermions in Optical Lattices

Principal Investigator: Nandini Trivedi

Department of Physics, The Ohio State University, 191 W. Woodruff Ave.,
Columbus, OH 43210. email: trivedi.15@osu.edu Tel: 614 247 7327

Co-Principal Investigator: Mohit Randeria

Department of Physics, The Ohio State University, 191 W. Woodruff Ave.,
Columbus, OH 43210. email: randeria.1@osu.edu Tel: 614 292 2457

Applicant Institution:

The Ohio State University Research Foundation, 1960 Kenny Road, Columbus, OH 43210.

ARO contact: Dr. Paul M. Baker,

Atomic and Molecular Program Manager, Army Research Office,
4300 S. Miami Blvd., Durham, NC 27703-9142
Phone: (919) 549-4202; Fax: (919) 549-4384; E-mail: Paul.M.Baker1@us.army.mil

1. Project Description

The study of strongly interacting Fermi systems using ultracold atomic gases has emerged as a major area of interdisciplinary research between atomic and molecular physics on the one hand and condensed matter physics on the other. This joining of hands has led and will lead to new advances in ideas, experiments and computational methods. In addition to its great intrinsic interest, this research on strongly interacting atomic gases is also expected to give insights into certain aspects of systems as diverse as high Tc superconductors, quark-gluon plasmas and color superconductivity in quantum chromodynamics.

There are many routes to achieving strong interactions in atomic gases, including, tuning the interaction using Feshbach resonances, quenching the kinetic energy via rapid rotation, and enhancing the potential to kinetic energy ratio using optical lattices. Here we will focus on optical lattices. The last several years have seen considerable activity in the field of strongly correlated bosons in optical lattices. The fermionic problem is only beginning to be studied experimentally and promises to be very exciting.

In this theory proposal we focused on addressing the question of strongly interacting fermions in optical lattices using a combination of quantum Monte Carlo simulations and analytical approaches. We modeled the systems by an effective low-energy Hamiltonian of the Hubbard form: a single band with an “on-site” attractive or repulsive interaction. In experiments this can be achieved by using laser fields which generate an optical lattice and staying far from Feshbach resonances. The lattice problem in the vicinity of a resonance is likely to involve occupation of higher bands and we avoided this complication since the single band problems are hard enough theoretically and rich enough to explore many important open questions.

(1.1) The big questions addressed in this proposal were:

How do many interacting particles organize themselves at low temperatures? Over the years many interesting phases have been revealed and it appears that the cold atom laboratory is ideal for finding some new exciting phases. We explored the emergence of new phases, and performed detailed quantitative simulations near the quantum phase transition to investigate the effects of strong repulsive and attractive interactions, population imbalance between fermion populations and thermal and quantum fluctuations near phase transitions. We successfully developed and applied a diverse set of numerical tools to investigate strongly correlated fermions optical lattices and in traps near quantum phase transitions.

1 Research Accomplishments from ARO Grant

A summary of the highlights of results in the area of optical lattice emulators obtained by the the PIs during the ARO grant (2008 - 2012) period have been:

- Bose superfluid-Mott insulator transition in optical lattices [1, 2]
- QMC simulations of the Fermi Hubbard model in 2D and 3D [6, 11]
- Spatially modulated FFLO pairing in spin-imbalanced fermions [3, 13]

and in strongly interacting fermions:

- BCS-BEC crossover and the unitary fermi gas [14, 9, 7]
- Contact, RF spectroscopy, and Viscosity [4, 5, 8]
- Upper branch of Feshbach resonance [10, 12]

Our ARO-funded work has had a major impact in the field. Our papers [1-15] include one publication in Proc. Nat. Acad. Sci. [10] and 4 Phys. Rev. Letters [1, 3, 6, 11]. In addition, we were invited to write a News and Views article in Nature Physics [9], a Perspective article to appear in Physics, and two long invited review articles on the BCS-BEC Crossover [14] and on the Hubbard model [15]. The two PI's have also been recognized by invited talks at major international conferences at KITP Santa Barbara (NT), KITP Beijing (NT), APS March Meeting (NT), INT Seattle (MR), CIFAR (MR) and Colloquiums at Harvard (MR), JILA (MR) and the Perimeter Institute (NT).

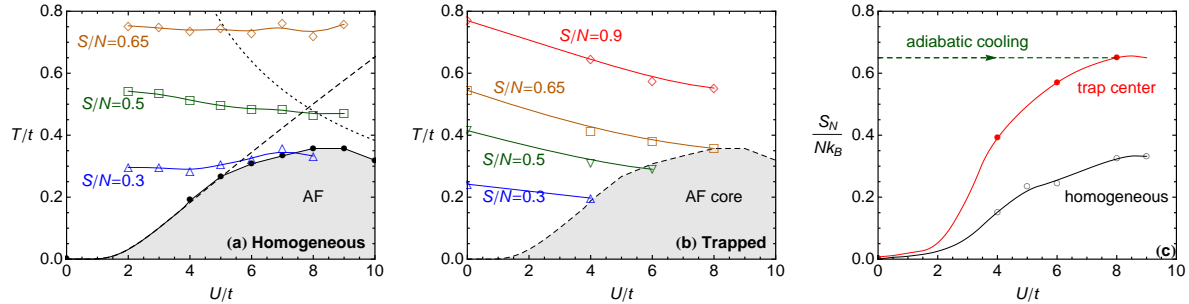


Figure 1: QMC plus LDA results on the 3D Fermi-Hubbard model [11]. (a) Constant-entropy curves of a homogeneous system at half-filling. There is no clear evidence for cooling as U is increased adiabatically, in marked contrast to (b). The filled symbols are QMC values for T_N ; the dashed and dotted curves are weak- and strong-coupling asymptotic forms. (b) In a harmonic trap with $E_t = 3.28t$, ramping up U adiabatically produces significant cooling due to entropy redistribution. An AF state can be produced at the trap center even for an overall entropy per particle $S/N \approx 0.65k_B$. (c) Average S/N in a harmonic trap below which AF order exists at the center. This is significantly higher than the critical S/N of a homogeneous system.

1.1 Optical lattices

Entropy and Cooling in Fermi Hubbard Model:

One of the major challenges in realizing antiferromagnetic (AF) and superfluid phases in optical lattices is the ability to cool fermions. We have used unbiased determinantal quantum Monte Carlo (QMC) simulations, free of the fermion sign problem, to examine the relevant temperature and entropy scales for the Fermi-Hubbard model in 2D [6] and in 3D [11]. We show [6] that an entropy per particle $S/N \simeq \ln 2$ is sufficient to observe the insulating gap in the 2D repulsive case at half-filling, or to see the pairing pseudogap in the 2D

attractive case. Observing AF correlations or superfluidity in 2D systems requires a further reduction in S/N by a factor of 3 or more. We also show that double-occupancy measurements are useful for thermometry for temperatures greater than the nearest-neighbor hopping energy.

We determine the equation of state for the 3D model [11] as a function of chemical potential, temperature, and repulsion using QMC, and use the local density approximation (LDA) to model a harmonic trap. In Fig. 1 we show that increasing repulsion leads to cooling but only in a trap, due to the redistribution of entropy from the center to the metallic wings. Thus, even when the average entropy per particle is larger than that required for AF in the homogeneous system, the trap enables the formation of an AF Mott phase.



Figure 2: **(Left) 3D Fermi-Hubbard model with spin imbalance** [3]: The mean-field phase diagram [3] with $U = -6t, T = 0$ in the (μ, h) plane. The dashed blue line corresponds to polarization $P = 0.37$. Also shown is a schematic of the corresponding shell structure in a harmonic trap within LDA. 80% of the atoms are in the LO phase. **(Right) Mapping the phase diagram of Bose Hubbard model** [1]: The local density $\rho^h(\mu(r))$ (purple), compressibility $\kappa^h(\mu(r))$ (red) and superfluid density $\rho_s^h(\mu(r))$ (blue) as functions of the radial coordinate in the trap. When finite ρ_s develops in some portion of the trap, $\kappa(r)$ shows sharp kinks coinciding with the S-N boundary. These kinks can be used to map out the phase boundaries of the homogeneous system.

Larkin-Ovchinnikov States for Imbalanced Fermi Gases in Optical Lattices:

The elusive Larkin-Ovchinnikov (LO) state with a modulated superfluid order parameter has long been sought in both imbalanced Fermi gases and in solid state materials. In Ref. [3] we show that the LO phase has a considerably larger range of stability in an optical lattice compared to the continuum. We obtain the phase diagram for the 3D attractive Hubbard model with spin imbalance using a fully self-consistent Bogoliubov-deGennes method. We find a strong modulation of the local polarization that should provide a distinct signature for detection of the LO phase. The shell structure in the presence of a trap generates singularities in the density at the phase boundaries that provide additional evidence for the LO phase. Depending on specific parameters, the LO ground state occurs over a large range of population imbalance, involving 80% of the atoms in the trap, and can exist up to an entropy $s = 0.5k_B$ per particle.

Bosons in Optical lattices:

Optical lattice experiments, with the unique potential of tuning interactions and density, have emerged as emulators of nontrivial theoretical models that are directly relevant for strongly correlated materials. Mapping out the finite temperature phase diagram for a strongly correlated quantum model remains a challenge. In Ref. [1] we propose a remarkable method for obtaining such a phase diagram directly from experiments using only the density profile in the trap as the input. We illustrate the procedure using the Bose Hubbard model, a textbook example of a quantum phase transition from a superfluid to a Mott insulator. Using exact QMC simulations in a trap with up to a 10^6 bosons, we show [1] that kinks in the local compressibility, arising from critical fluctuations, demarcate the boundaries between superfluid and normal phases in the trap. The temperature of the bosons in the optical lattice is determined from the density profile at the edge. Our method can be applied to other phase transitions even when reliable numerical results are not available.

In Ref. [2], we develop a strong-coupling expansion for the momentum distribution of the Bose Hubbard model, whose results are benchmarked against numerically exact QMC simulations in 2D and 3D and against DMRG calculations in 1D. We expect that these analytical results will be useful for easy comparison with experiments and can, in some cases, bypass the need for expensive numerical simulations.

1.2 Strongly Interacting Fermi Gases:

The PIs have earlier made pioneering contributions to the problem of BCS-BEC crossover starting in the 1990's, including the prediction of the pairing pseudo gap in the strongly interacting regime. Our recent contributions have focused on the unitary regime where the s -wave scattering length becomes infinite. In the past few years we have obtained important results on the universal high frequency behavior of dynamical correlations [4, 5, 8], sum rules for viscosity [8] and the role of quantum fluctuations [7]. These results are summarized below. Our theoretical predictions [4, 5] for the back-bending in angle-resolved RF spectra and of the $C\omega^{-3/2}$ tail in RF spectra have both been verified experimentally in D. Jin's group at JILA. Understanding the large- k back-bending in RF spectra is crucial to the proper identification of near- k_F pseudo gap, and the RF tail has been used extensively to measure the contact C .

A new direction in our research, motivated by various experiments at MIT, is that of fermions on the repulsive branch of Feshbach resonance [10, 12]. These results are briefly mentioned below and discussed further in Sec. 3.3, where we take up related questions in our proposed research.

RF Spectroscopy of strongly interacting fermions:

We have elucidated the universal short-distance structure of the single-particle spectral function of Fermi gases [4] and discussed how it leads to surprising observable features in RF and angle-resolved RF experiments. We show that the Tan's universal C/k^4 tail in the momentum distribution implies that the spectral function $A(\mathbf{k}, \omega)$ *must* have weight below the chemical potential, for large momentum $k \gg k_F$, which can be probed RF spectroscopy experiments. We find that this incoherent spectral weight is centered around $\omega \simeq -\epsilon(k)$ in a range of energies of order $v_F k$. This universal “bending back” of the dispersion, while natural for superfluids, is quite surprising for normal gases. We argue that, even in superfluid or pseudogap state, this bending back at large k is dominated by interaction effects which do not reflect the pairing gap.

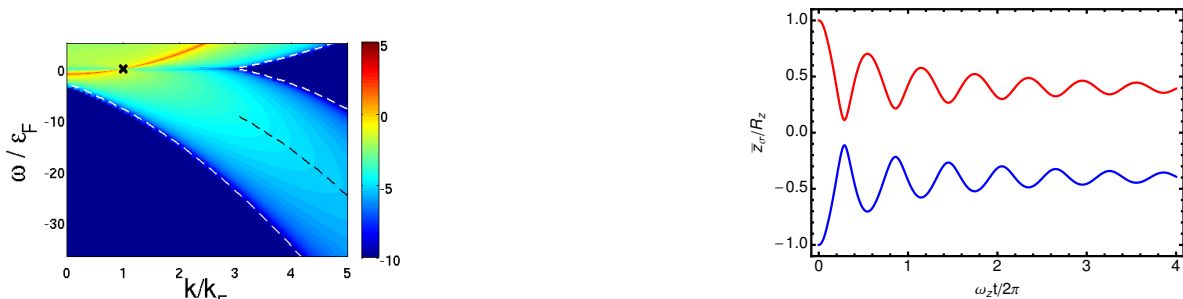


Figure 3: **(Left) Universal back-bending in angle-resolved RF spectral function** [4]: Logarithmic intensity plot of $A(k, \omega)$ of a repulsive Fermi gas showing incoherent spectral weight at large $k \gg k_F$ centered around $\omega \simeq -k^2/2m$ with an integrated intensity of C/k^4 . **(Right) Collision of spin-polarized clouds** [12]: Time dependence of the center-of-mass positions of the two clouds at unitarity, with the red (upper) and blue (lower) curves denoting the center of mass of the two spin species. The calculation, based on hydrodynamics with an upper branch energy functional, shows a “bounce” at small times followed by a “phase segregation” regime, where the two center-of-masses remain at a constant separation.

Viscosity, spectral functions and sum rules:

In Ref. [8] above we gave the first derivation of sum rules for the frequency-dependent shear and bulk viscosity spectral function in quantum fluids. These sum rules enabled us to derive several exact results for strongly interacting Fermi gases. Notably, that the bulk viscosity in a unitary Fermi gas vanishes

identically for all frequencies and all temperatures. We also used our sum rules to determine the exact form of high-frequency tails in the spectral functions and in the dynamic structure factor. Finally, we predict that frequency-dependent shear viscosity of the unitary Fermi gas can be experimentally measured using two-photon Bragg spectroscopy.

Sum rules are exact results valid even in regimes where strong correlations make standard calculations unreliable. As such, they are crucial for analyzing experimental data and constraining numerical calculations. Recently, there has been considerable interest in the viscosity of strongly interacting quantum liquids owing to conjecture based on a string theory (AdS-CFT) calculation that the viscosity divided by entropy is bounded from below. Only systems with very strong interactions are capable of saturating this bound. Experimentally, it has been established that the unitary Fermi gas and the quark-gluon plasma produced at the Relativistic Heavy-Ion collider (RHIC) are the only systems which come close to saturating this bound. Our sum rules suggest close similarities between the unitary Fermi gas, quark-gluon plasma and the system for which the initial AdS-CFT calculation was performed. These systems have in common the feature that they are all strongly-interacting, with no sharp quasiparticles.

BCS-BEC crossover with unequal mass fermions:

In ref. [7], we have investigated the BCS-BEC crossover with two fermion species with different masses M and m interacting via a Feshbach resonance. We compute the $T = 0$ equation of state as a function of the scattering length, including effects of Gaussian fluctuations [16] about mean field theory. The ground state energy as a function of M/m at unitarity is in excellent agreement with available QMC results for ^{40}K - ^6Li mixtures. The dimer scattering length in the BEC limit as a function of M/m compares well with exact four-body results.

Strongly interacting fermions on the upper branch:

We address the question of ferromagnetism in repulsive Fermi gas, a problem of fundamental interest, using QMC simulations that include backflow corrections [10]. We investigate a two-component Fermi gas on the upper branch of a Feshbach resonance, motivated by recent experiments [102], and contrast it with the text-book problem hard-sphere gas. The latter had not been solved with state of the art QMC methods until our work [10] and ref. [107]. We find that, in both cases, the Fermi liquid becomes unstable to ferromagnetism at a $k_F a$ smaller than the mean field result. Even though the total energies are similar in the two cases, their pair correlations and kinetic energies are completely different, reflecting the underlying potentials. Our analysis of the upper branch simply assumes that the system is stable, an assumption that may not be justified by later experimental developments [103]. We propose to explore this question further as described in detail in Sec. 3.3.

Motivated by a recent experiment at MIT [123], we consider the collision of two clouds of spin-polarized atomic Fermi gases close to a Feshbach resonance. We explain why two dilute gas clouds, with underlying attractive interactions between its constituents, bounce off each other in the strongly interacting regime. Our hydrodynamic analysis, in excellent agreement with experiment, gives strong evidence for a novel metastable many-body state with effective repulsive interactions.

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